Determination of Structural and Possible Ferromagnetic Properties of $Cr_xSn_{1-x}O_2$ Compounds: First Principle Approach

Ayedun, F.
Department of Physics, National Open University of Nigeria, Abuja
Corresponding author: fayedun@noun.edu.ng

ABSTRACT: The total energy calculations of structural and magnetic properties of a six atom supercell of pure, binary, tetragonal structure SnO_2 at x =0 and twelve atom supercells of ternary transition metal oxides $Cr_xSn_{1-x}O_2$ at x =0.25, 0.50, 0.75 and 1.00 were simulated using first-principles calculations within the framework of generalized gradient approximation (GGA) for spintronic utilities. Doping Cr with wide band gap SnO_2 has the effect of transition from a non-mental to metallic state.The calculated magnetic moment at x = 0.25 is 1.9976 μB, x = 0.50 is 3.9309 μB,x=0.75 is 5.8831 μB and x=1.00 is 7.8271 μB. The room temperature ferromagnetism attained in this study is apparent in Sn substitution with Cr atom.

KEYWORDS: Ferromagnetic, Diluted semiconductor, Metal oxides, Spintronic devices.

1. INTRODUCTION

Dilute magnetic semiconductor is a non-magnetic semiconductor doped with magnetic atoms most especially transition metals to induce magnetic and spin-polarized materials which exhibits both ferromagnetism and semiconductor properties. It's of interest because of its functionality in the development of spintronic devices. The substituted Cr^{2+} ions has magnetic moment attribute into Sn^{2+} ions in $Cr_xSn_{1-x}O_2$ at various compositions; x=0.25, 0.50, 0.75 and 1.00 respectively without having any negative consequence on the resulting structure of CrO_2 at x=1.00.

Tin oxide(SnO_2) is a wide band gap semiconductor oxide and is useful in magnetic data storage and resonance imaging, photo catalyst (Pearton et. al., 2003), increase refractoriness (Jednak et al., 2011), electrodes and anti-reflection coatings in solar cells (Wolf et al.,2001), manufacturing of gas sensors, optoelectronic devices and resistor (Al-Saadi et al., 2019), polishing powder, glass coatings and making of liquid crystal display and so on.

Chromium(IV) oxide (CrO_2) is metastable at room temperature and pressure and is of interest as a result of its potential usage in spintronic heterostructures, superconductor structures (Anwar et al, 2010), electronic storage device, catalyst and corrosion inhibition devices, magnetic heads and magnetic field sensors (Bate, 1978) polishing agents medicine, (Kurmaev et al., 2003) to mention a few. Transition metal oxide,SnO_2doped with Cr atom finds usefulness in production of riboflavin biosensors (Lavanya, 2013), processing of pigments, gas sensors and optional applications. The spin and orbital magnetic moments of Cr and O in CrO_2 usinglocal spin density approximation (LSDA) approach was reported (Jeng and Guo, 2002). The computed sub-lattice magnetic moment of Cr in rutile-type $CrO_2$of 2.04 μB was deducted (Huang et al., 2018).

Ferromagnetism entails magnetic ordering in which the intrinsic magnetic dipole moment or spin of electrons on each crystal-lattice site all align in the same direction. The two unique features of ferromagnetic are: spontaneous

magnetization of which the total magnetization exists within a uniformly magnetized microscopic volume without the presence of a field and magnetic ordering temperature. Ferromagnets either possess strong attractive or repulsive forces in the presence of permanent magnet (Aibangbee and Onohaebi, 2018). Utilization of ferromagnetism are: data storage, electromagnets, magnetic tape recording and transformers (Hummel, 2013).

There have been considerable studies of Cr doped semiconductor, SnO_2both experimental and theoretical wise (Stashans et al., 2014, Kuppan et al., 2017, Mishra et al., 2015) with various methodologies (Abidi et al., 2013, Leite et al.,2005 and Kasar et al., 2013). Albeit, there is need to study the effects of chromium doped semiconductor material SnO_2at x=0.25, 0.50, 0.75 and 1.00 using PBE-PAW technique and density functional theory based so as to understand its structural and room temperature magnetic properties as an effective gas sensor on ceramic materials.

2. COMPUTATIONAL DETAILS AND THEORETICAL BACKGROUND

The appraisals of this study were actualized by using Perdew-Burke- Ernzhof Projected Augmented wave within the framework of Generalized Gradient Approximation (GGA) based density functional theory and Perdew-Burke-Ernzhof Projected Augmented Wave (PBE- PAW) technique (Ayedun et al., 2017). The PBE- PAW approach is preferred in this work because it enhances adequate and accurate facts about equilibrium state, structural minimization, response, spectroscopic and magnetic properties of crystalline structures and so on. Also, PBE- PAW technique (Perdew et al., 1997) is time and cost effective, accurate pseudopotential libraries are highly available and accessible in the Quantum Espresso package (Giannozzi et al., 2009). $Cr_x\,Sn_{1-x}O_2$ retainsits crystalline tetragonal structure from compositions x = 0 to 1. The details of volume (V)-energy (E) were fixed in the second –order Birch-Murnaghan equation of state (Birch, 1994; Murnaghan, 1994) and minimized lattice parameters a and c (since a = b, but b ≠ c) at room temperature were examined.

$$\delta E(V) = E - E_0 = BV_0\left[\frac{V_n}{B'}\right] + \left(\frac{1}{\left(1-B'\right)}\right) + \left(\frac{V_n}{B'\left(B'-1\right)}\right). \quad \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

The plane wave cut-off energy is set at 80 Ry for a K- mesh of 10 x 10 x 5 for a pure six atom supercell, SnO_2. The Monkhorst – Pack (Monkhorst and Park, 1976) K-meshes of 10 x 10 x 5, 8 x 8 x 4, 10 x 10 x 5 and 10 x 10 x 5 for a twelve atom supercell built and kinetic energy of 90 eV each were set at x = 0.25 to 1.00 respectively. Self consistent relaxation of atomic positions were quantumly simulated and the optimized energy converged to 0.01 milli electronVolt (meV) at each concentration x in respect of Brillouin zone and cut – off energy. Comparison is made with existing experimental and theoretical works via calculations performed in non-defective SnO_2 at x = 0 and doped ternary compounds of $Cr_x\,Sn_{1-x}O_2$ at x = 0.25 to 1.00, with minimized structural parameters of a and c as indicated in Table 1.

Table 1: Optical lattice parameters of $Cr_x\,Sn_{1-x}O_2$ compound.

Parameter(Å)	**Present Study**	**Existing Works**	
		Experimental	**Theoretical**
a	4.7358	4.743, 4.7202, 4.7471	4.8959, 4.780
c	3.1853	3.2070, 3.200	3.30371, 3.268

The values of optimized lattice parameters enlisted in Table 1 are in conformity with existing experimental and theoretical studies (ESI, 2013).

3. RESULTS AND DISCUSSION

3.1 Structural Properties

The pattern of undoped (six atoms supercell), binary rutile SnO_2 and doped ternary transition metal oxides (twelve atoms supercell) $Cr_x\,Sn_{1-x}O_2$ at concentrations x = 0.25 to 1.00 remains tetragonal rutile body centered cubic structure. The details of volume (V) – Energy (E) were imputed in the second order Birch- Murnaghan equation of state (Birch, 1947; Murnaghan, 1947) and minimized lattice parameter a, bulk modulus B and pressure derivative B' at room temperature were determined. Vegard's law examined the rules of mixture using lattice parameter of a solid solution of two constituents A and B at constant temperature and uniform crystal structure. This law is not limited to only pure binary solid solution A and B, it is also applicable to ternary transition metallic oxide, $Cr_x\,Sn_{1-x}O_2$. The lattice parameter as attested by Vergard's law is:

$$a\left(A_x\ B_{1-x}\ C\right) \quad = \quad x\,a_{AC} + (1-x)\,a_{BC}, \quad \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots (2)$$

herein, a_{AC} and a_{BC} are the equilibrium lattice constants of CrO_2, SnO_2 and $a\left(A_x\ B_{1-x}\ C\right)$ is the ternary compound lattice constant, x is the molar fraction of Cr in SnO_2 for $0 \angle x \angle 1$. Because of lack of compliance to Vergard's law in semiconductors both theoretical (Ayedun, 2017, Abdiche, 2010) and experimental works (Gu et al., 2007; Wei et al., 2020;Savidan et al., 2010) can now be written as:

$$a\left(A_x\ B_{1-x}\ C\right) \quad = \quad x\,a_{AC} + (1-x)\,a_{BC} \quad - x\,(1-x)\,b, \quad \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots (3)$$

where b stands for bowing constant.The substitution of Sn with Cr atoms at x =1, results into mini overvalue of lattice constant and a better transition compound produced. The lattice parameter of undiluted SnO_2 at x = 0(4.7358 Å) and that of alloyed transition metal oxide at x =1(4.6442 Å) are very close as revealed in Table2.

Table 2: Lattice parameter a, bulk modulus B and pressure derivative B' of $Cr_x\,Sn_{1-x}O_2$ compound

Nomenclature	Parameters	Present Study	Experimental Values	Theoretical Data
SnO_2	A (Å) B (GPa) B' (GPa)	4.7358 413.0 9.63	4.743, 4.7202277 2.0	4.8959, 4.780312
$Cr_{0.25}Sn_{0.75}O_2$	A (Å) B (GPa) B' (GPa)	4.7834 577.1 15.0	-	-
$Cr_{0.50}Sn_{0.50}O_2$	A (Å) B (GPa) B' (GPa)	4.7777 663.2 15.0	-	-
$Cr_{0.75}Sn_{0.25}O_2$	A (Å) B (GPa) B' (GPa)	4.7305 907.7 14.48	-	-
CrO_2	A (Å) B (GPa) B' (GPa)	4.6442 660.1 3.62	4.421 239	4.384, 4.459 237.7

The component of chromium compositions modification with lattice constant and bulk modulus were considered. The calculated optimized lattice constants were plotted against chromium compositions(x) in Figure 1. As the chromium dopant increases from x = 0 to 1.00, the downward bowing constant of ternary compound $Cr_x\,Sn_{1-x}O_2$ is -0.34. The difference in lattice constant at x = 1(4.6442 Å) compared with that of existing theoretical data (4.384 Å and 4.459Å)by Srivastav et al., 2008 and Huang et al., 2018 respectively, depicted in Table 2 is as aresult of GGA artefact used.

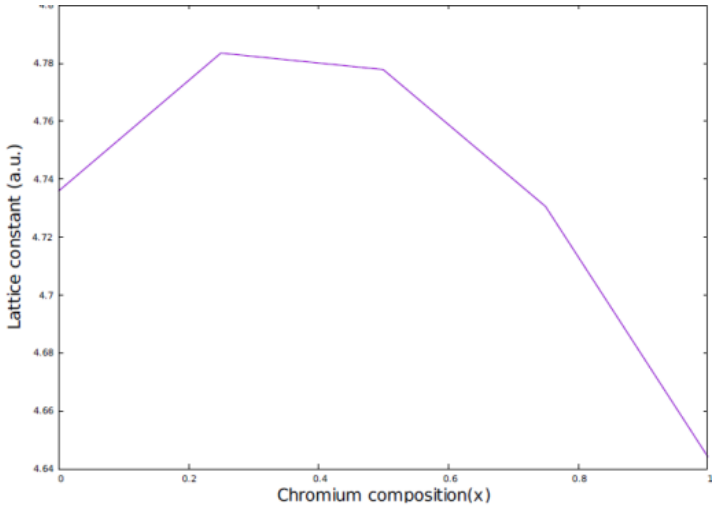

Figure 1: Lattice constant of $Cr_x\,Sn_{1-x}O_2$ as function of chromium composition (x)

The bulk modulus varies with rising chromium composition from x = 0.25 to 0.75 and decrease to 660.1 GPa at x = 1.00 as indicated in Figure 2. The increase in bulk modulus is due to the fact that GGA has tendency to overestimate and the bulk modulus bowing constant is -0.90.

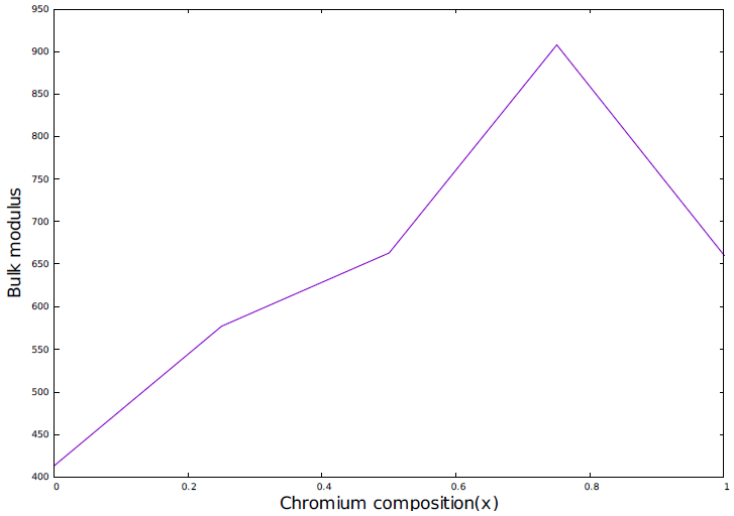

Figure 2: Bulk modulus of $Cr_x\ Sn_{1-x}O_2$ as function of chromium composition (x)

3.2Magnetic Properties

Magnet has the capacity to create magnetic field. Magnetic field is produced as much as orbits are set in motion as well as there exist the spinning of electrons. The three major types of magnet are electromagnet, permanent magnet and temporary magnet. The feature of magnet comprises of its attractive property, directive property, pair property to mention a few. Magnets are grouped into diamagnetic, paramagnetic, ferromagnetic, ferrimagnetic antiferromagnetic. The magnitude of magnetic moment which quantifies the magnetic properties of material is a function of an unpaired electron. At x = 0, $SnO_2$is diamagnetic because both $Sn^{2+}$and O^{2-} are paired and the net magnetic field effect is zero (Wang et al., 2010). The outer valence electrons; $Sn\left(4d^{10}5s^2\,5p^2\right)$, $Cr\left(3s^2 3p^6\,3d^4\right)$, $O\left(2s^2 2p^4\right)$ which are unpaired enhanced increase in magnetic moment as dopant atom, chromium increases from x = 0.25 to 1.00. The bulk magnetic moment of $Cr_x\ Sn_{1-x}O_2$ compounds were examined at x =0 to x = 1.00 as shown in Table3.

Table 3: Magnetic moment of $Cr_x\ Sn_{1-x}O_2$ compound in μB.

Composition (x)	Nomenclature	Present study	Experimental	Theoretical
0	SnO_2	0	0	0
0.25	$Cr_{0.25}Sn_{0.75}O_2$	1.9976	-	-
0.50	$Cr_{0.50}Sn_{0.50}O_2$	3.9309	-	-
0.75	$Cr_{0.75}Sn_{0.25}O_2$	5.8831	-	-
1.00	CrO_2	7.8271	-	9.0

Magnetic moment increased linearly with risen chromium atom substitution as displayed in Figure 3. A weak ferromagnetic (1.9976 μB) was observed at x = 0.25 and a strong ferromagnetic material emerged at x = 1(7.8271 μB).

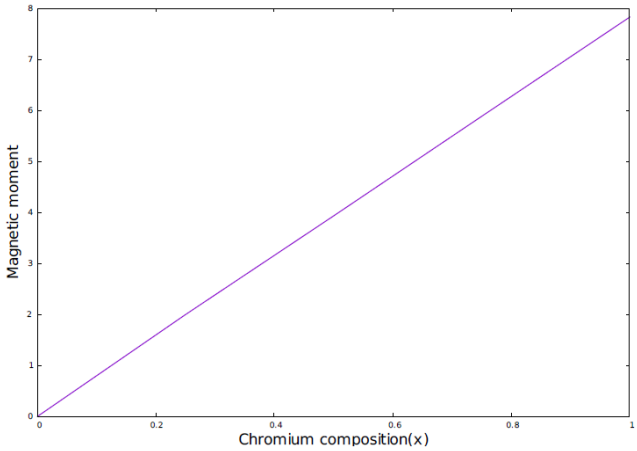

Figure 3: Magnetic moment of $Cr_x Sn_{1-x} O_2$ as function of chromium composition (x)

4. CONCLUSION

Cr atom was substituted into $Cr_x Sn_{1-x} O_2$ ternary compound at various composition x = 0 to 1.00 using PBE-PAW approach. The addition of the dopant increased the lattice parameter, enhanced the pressure as well as the bulk modulus. It influenced the phase transition from nonmagnetic material SnO_2 to room temperature ferromagnetic system at x = 0.25 to 1.00 without distortion to its tetragonal rutile structure. The researchers are recommended to experimentally work on the bulk magnetic moment of SnO_2 with transition metals using various methodologies.

REFERENCES

Abdi, M. H., Ibrahim, N. B., Mohagheghee, M. M. B. (2013). Deposition andcharacterization of chromium doped tin oxide transparent conducting thin films preparedbyspray pyrolysis technique. *Applied Mechanics and Materials*, 313, 164-168. DOI:10.4028/www.scientific.net/AMM.313-314.164.

Abdiche, A. Abid, H., Riane, R., Bouaza, A. (2010). First-principles study of cubic $B_x In_{1-x} N$ Ternary Alloys. *Acta Physica Polonica A*, 117, 921-927.

Aibangbee, J. O., Onohaebi, O. (2018). Ferromagnetic materials characteristics: Their application in magnetic cores using Hysteresis loop measurements. *American Journal of Engineering Research*, 7(7)**,**113-119. https://www.ajer.org/papers/Vol-7-issue-7/L0707113119.pdf (4).

Alptekin, S. (2015). Pressure-induced phase transformation in CrO_2. *Journal of Molecular Modeling*. DOI:10.1007/s00894-015-2852-5.

Al-Saadi, T. M., Hussein, B. H., Hasan, A. B., Shehab, A. A. (2019). Study the structural andoptical properties of Cr doped SnO_2 nanoparticles synthesized by Sol- Gel method. *Energy Procedia*, 157, 457-465.

Anwar, M. S., Czeschka, F. Porcu, M., Aarts, J. (2010). Long-range super currents through half-metallic ferromagnetic CrO_2. *Physical Review B*, 82, 100501,https://link.aps.org/doi/10.1103/PhysRevB.82.100501.

Ayedun, F., A.debambo, P.O., Adetunji, B. I., Ozebo, V. C., Oguntuase, J. A., Adebayo, G.A. (2017). Increased

malleability in tetragonal $Zr_x Ti_{1-x} O_2$ ternary alloys: first-principlesapproach. *Zeitschrift fur Naturforschung A*, 72(6), 1-6,https://doi.org/10.1515/zna-2017-0036.

Bate, G. A. (1978). A survey of recent advances in magnetic recording materials. *IEEE Transactions on Magnetic*, 14 (4)**,** 136-142. **DOI:**10.1109/TMAG.1978.1059769.

Birch, F. (1947).Finite elastic strain of cubic crystals. *Physical review 71*, 809-824. https://link.aps.org/doi/10.1103/PhysRev.71.809

ESI (2013). Electronic Supplementary Material for Physical Chemistry.*Chemical Physics*. The Owner Societies.

Fitzgerald, C. B., Venkatesan, M., Dorneles, L. S., Gunning, R., Stamenov, P., Coey, J. M. D., Stampe, P. A., Kennedy, R. J., Moreira, E. C., Sias, U. S. (2006). Magnetism in dilute magnetic oxide thin films based on SnO_2. *Physical Review B*, 74 (11), https://link.aps.org/pdf/10.1103/PhysRevB.74.115307

Giannozzi, P., Baroni, S., Bonini, N., Calandra, M., Car, R.., Cavazzoni, C., Cersoli, D., Charotti, G. L., Cococcioni, M., Dabo, I., Dal Corso, A., Gironcoli, S. de., Fabris, S., Fratesi, G., Gebauer, R.., Gerstmann, U., Gougoussis, C., Kokalj, A., Lazzeri, M., Martin-Samos, L., Marzari, N., Mauri, F., Mazzarello, R., Paolini, S., Pasquarello, A., Paulatto, L., Sbraccia, C., Scandolo, S., Sclauzero, G., Seitsonen, A.P., Smogunov, A., Umari, P., Wentzcovitch, R. M. (2009). *Journal of Physics: Condensed Matter*, 21, 395502, doi: 10.1088/0953-8984/21/39/395502.

Gracia, L., Beltran, A., Andres, J. (2007). Characterization of the high-pressure structures and phase transformations in SnO_2. A density functional theory study. *The journal of physical chemistry*. doi: 10.1021/jp067443v

Gu, Z. F., Xu, C.F., Cheng, G., Jiang, M. H., Wang, Z. M., Zhou, H. Y., Liu, X. M., Lin, Y. Y. (2007). Experimental study of ternary Nd-Pt-Fe phase equilibria at 500ºC. *Material Science and Technology*, 23 (12)**,**1492-1496. https://doi.org/10.1179/174328407X2486_13

Gul, R.., Victor, M. G., Soon, C.H. (2008). Vacancy-induced magnetism in SnO_2: A density functional study. *Physical Review B*, 78, 184404. https://link.aps.org/doi/10.1103/PhysRevB.78.184404

Huang, S., Wu, X., Niua, J., Qin, S. (2018). Structural, magnetic and electronic properties of CrO_2 at multimegabar pressures. *RSC Advances*, 43, 24561-24570.

Hummel, R. E. (2013). Electronic properties of materials. Springer New York, 347-371.

Jedynak, L., Wojsa, J., Podworny, J., Wala, T. (2011). Refractories from the $MgO\text{-}Al_2O_3\text{-}SnO_2$ system for metallurgical applications. *Ceramic Materials*, 63 (1), 34-39.

Jeng, H., Guo, G. Y. (2002). First-principles investigations of the orbital magnetic moments in CrO_2. *Journal of Applied Physics*, 92(2), 951-957, https://doi.org/10.1063/1.1486260

Kasar, R. R.., Gosavi, S. R.., Ghosh, A., Deshpande, N. G., Sharma, R. P. (2013). Influence of Cr doping on structural, morphological and optical propertiesof SnO_2 thin film prepared by spray pyroylysis technique, *IOSRJournal of Applied Physics*, 7, 21 -26.

Kholiya, K., Pandey, K. (2019). High pressure compression behavior of bulk and nanocrystalline SnO_2. *Journal of Taibah University for Science*, 13(1), 592-596, https://doi.org/10.1080/16583655.2019.1611369

Kuppan, M., Babu, S. H., Kaleemulla, S., Madhusudhanarao, N., Krishnamoorthi, C., Venugopalrao, G., Omkaram,

I., Reddy, D. S., Reddy, V. S. (2017). Structural and magnetic properties of Cr doped SnO_2 nanopowders pepared by solid state reaction. Mechanics, Materials Science and Engineering **9**, ISSN 2412-59542.

Kurmaev, Z., Moewe, A., Butorin, S. M., Katsnelson, M. I., Finkelstein, L. D., Nordgren, J., Tedrow, P. M. (2003). Half-metallic electronic structure of CrO_2 in resonant scattering. *Physical Review B*, 67, 155105-155109, DOI:10.1103/PhysRevB.67.155105

Lavanya, N., Radhakrishnan, S. J., Sekar, C., Navaneethan, M., Hayakawa, Y., Nordgren, J., Tedrow, P. M. (2013). Fabrication of Cr doped SnO_2 nanoparticles based biosensor for the selective determination of riboflavin in pharmaceuticals. *The Analyst*, 138(7), 2061-2067, doi:10.1039/c3an36754a

Leger, H. (1993). Phase transitions in ruthenium dioxide up to 40 GPa: Mechanism for the rutile-to-fluorite phase transformation and a model for the high-pressure behavior of stishovite SiO_2. *Physical Review B, Condensed Matter*. Doi:10.1103/PhysRevB.48.13344

Leite, D. R., Las, W. C., Brankovic, G., Zaghete, M. A., Cilense, M., Varela., J. A. (2005). Use of impedance spectroscopy in the study of the effect of Cr concentration on the electrical properties of SnO_2-based ceramics. *Materials Science Forum*, 498-499, 337-341, DOI:10.4028/www.scientific.net/AMM.313-314.164

Letifi, H., Litaiem, Y., Dridi, D., Ammar, S., Chtourou, R. (2019). Enhanced Photocatalytic Activity of Vanadium-Doped SnO_2 Nanoparticles in Rhodamine B Degradation. *Advances in Condensed Matter Physics*. https://doi.org/10.1155/2019/2157428

Maddox, B. R., Yoo, C. S., Kasinathan, D., Pickett, W. E., Scalettar, R. T. (2006). High-pressure structure of half-metallic CrO_2. *Physical Review B*, 73, 144111. DOI: https://doi.org/10.1103/PhysRevB.73.144111.

Mishra, R. K., Kushwaha, A., Sahay, P. P. (2015). Cr-induced modifications in the structural, photoluminescence and acetone-sensing behavior of hydrothermally synthesized SnO_2 nanoparticles. Journal of Experimental Nanoscience **10(13),** 1041-1056, DOI:10.1080/17458080.2014.952685

Monkhorst, H. J., Pack, J. D. (1976). *Physical Review B*, 13, 5188-5192. http://dx.doi.org/10.1103/PhysRevB

Murnaghan, F. D. (1944). The compressibility of media under extreme pressures. *Proc Natl Acad Sci USA.*, 244-247 https://doi.org/10.1073/pnas.30.9.244

Pearton, S. J., Abernathy, C. R.., Thaler, G. T., Frazier, R.., Ren, F., Hebard, A. F., Park, Y. D.; Norton, D. P., Tang, W.; Stavola, M.; Zavada, J. M. and Wilson, R. G. (2003). Effects of defects and doping on wide band gap ferromagnetic semiconductors, *Physica B*, 340, 39 –47, doi:10.1016/j.physb.2003.09.003

Perdew, J. P.; Burke, K. Ernzehof, M. (1997). Generalized gradient approximation made simple. *Physical Review Letters*, 77, 3865-3868, DOI:https://doi.org/10.1103/PhysRevLett.78.1396. *Erratum Physical Review Letters*, 78, 1396.

Ponce, C. A., Caravaca, M. A., Casali, R. A. (2014). Mechanical anisotropy and thermoacoustic properties of SnO_2 under high pressures: an ab initio approach. *High Pressure Research*, 34(2). https://doi.org/10.1080/08957959.2013.867041

Rahman, G., Garcia-Suarez, V. M., Hong, S. C. (2008). Vacancy-induced magnetism in SnO_2: A density functional study. *Physical Review B 78*, 184404-184409, DOI:10.1103/PhysRevB.78.184404.

Savidan, J. C., Joubert. J. M., Toffolon-Masclet (2010). An experimental study of the Fe-Sn-Zr ternary system at 900ºC. *Intermetallics*, 18(11), 2224-2228. ISSN: 0966-9795.

Srivastava, V., Rajagopala, M., Sanyal, S. P. (2008). First principles study of structural, magnetic and electronic properties of half-metallic CrO_2 under pressure. *The European Physical Journal B,* 61, 131-139.

Stashans, A., Puchaicela, P., Rivera, R. (2014). DFT study of chromium-doped SnO_2 materials. *Journal of Material Science*, 49, 2904-2911.

Wang, C., Ge, M., Jiang, J. Z. (2010). Magnetic behavior of SiO_2 nanosheets at room temperature. *Applied Physics Letters*, 97, 042510-042513. https://doi.org/10.1063/1.3473764

Wei, Q., Lu, Z., Wang, J., Yao, Q., Long, Q., Qin M., Zhou, H. (2020). Experimental Investigation of phase Equilibria in the La-Fe-B System at 600º and 800ºC. *Journal of Phase Equilibria and Diffusion*, 41, 35-43.

Wolf, S. A., Awschalom, D. D., Buhrman, R. A., Daughton, J. M., von Molnar, S., Roukes, M. L., Chtchelkanova, A. Y. and Treger, D. M. (2001). Spintronics: A Spin-Based Electronics Vision for the Future. *Science*, 294, 1488-1495, doi:10.1126/science.1065389.